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MCNPX VERSION 2.5.c

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MCNPX VERSION 2.5.C

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Executive Summary

MCNPX is a Fortran 90 Monte Carlo radiation transport computer code that transports all particles at all energies. It is a superset of MCNP4C3, and has many capabilities beyond MCNP4C3. These capabilities are summarized along with their quality guarantee and code availability. Then the user interface changes from MCNP are described. Finally, the new capabilities of the latest version, MCNPX 2.5.c, are documented. Future plans and references are also provided.

1.0. INTRODUCTION

MCNPX is a Fortran 90 Monte Carlo radiation transport computer code that transports all particles at all energies. MCNPX stands for MCNP eXtended. It is a superset of MCNP4C3, and has many capabilities beyond MCNP4C3. MCNPX is a production computer code for modeling the interaction of radiation with matter, and its quality is guaranteed: it can be used with confidence. MCNPX is available from RSICC and OECD/NEA; beta test program versions may be downloaded from the MCNPX website, http://mcnpx.lanl.gov.

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1.1. MCNPX Capabilities Beyond MCNP4C3

Each successive version of MCNPX adds new capabilities and modernizes the code for new hardware, operating systems, and compilers. The capabilities of MCNPX beyond MCNP4C3 are now listed, grouped according to MCNPX version. Initials of principal developers are shown in parentheses.¹ For completeness we also list the capabilities and principal developers of MCNP and MCNPX since MCNP4B.

MCNPX 2.5.c (April 2003)

MPI multiprocessing (JL/GWM);
I,J,K lattice indexing in geometry plots (JSH),
Enable weight window generator in physics model region (FXG/JSH);
Enable exponential transform in physics model region (FXG/JSH);
Extend neutron model physics below 20-MeV (JSH);
3-He coincidence detector modeling (HGH/JSH);
F90 Autoconfiguration (TLR);

¹ Kenneth J. Adams (KJA), Leland L. Carter (LLC), Skip Egdorf (HWE), Thomas J. Evans (TJE), Jeffrey A. Favorite (JAF), Franz X. Gallmeier (FXG), John S. Hendricks (JSH), H. Grady Hughes (HGH), Julian Lebenhaft(JL), Robert C. Little (RCL), Stepan G. Mashnik (SJM), Gregg W. McKinney (GWM), Richard E. Prael (REP), Teresa L. Roberts (TLR), Arnold J. Sierk (AJS), Edward C. Snow (ECS), Laurie S. Waters (LSW), Christopher J. Werner (CJW), and Morgan C. White (MCW).

	Corrections/enhancements/extensions.
MCNPX 2	2.5.b (November 2002)
	CEM2k physics (SGM/AJS/FXG); Mix and Match (JSH); Positron Sources (HGH); Spontaneous Fission (JSH); Corrections/enhancements/extensions.
MCNPX 2	2.4.0 (August 2002)
	FORTRAN 90 modularity and dynamic memory allocation (GWM); Distributed memory multiprocessing for the entire energy range of all particles (GWM); Repeated structures source path improvement (LLC/JSH); Default dose functions (LSW/JSH); Light-ion recoil (JSH); Enhanced color geometry plots (GWM/JSH); Photonuclear cross-section plots (JSH); Proton cross-section plots (JSH); Proton reaction multipliers with FM cards (JSH); Photonuclear reaction multipliers with FM cards (JSH/GWM); Some speedups (GWM/JSH); Logarithmic interpolation on input cards (JSH); Cosine bins that may be specified in degrees (JSH); Cosine bins may be specified for F2 flux tallies (JSH); Source particles that may be specified by descriptors (JSH); Pause command for tally and cross-section plots (JSH); and Correction of all known MCNPX and MCNP4C bugs/problems.
MCNPX 2	2.3.0 and previous MCNPX versions (1995-2001)
	Physics for 34 particle types (HGH); High-energy physics above the tabular data range (REP); Photonuclear physics (MCW); Neutron, proton, and photonuclear 150-MeV libraries and utilization (RCL); Mesh tallies (tally in a superimposed mesh) (LSW/ECS); Radiography tallies (JSH/ECS); Secondary-particle production biasing (ECS); and Autoconfiguration build system for compilation (TLR/HWE).

MCNP4C3, MCNP4C2, and MCNP4C features added after MCNP4B (1997-2001)
 □ PC enhancements: Linux and Windows capable (LLC/GWM);
 □ Easier geometry specification with macrobodies (LLC);
 □ Interactive geometry plotting (JSH);
 □ Improved variance reduction with the superimposed mesh weight window generator (TME/JAF/JSH);
 □ Superimposed mesh plotting (JSH);
 □ Delayed neutrons (CJW);
 □ Unresolved resonance range probability tables (LLC/RCL);
 □ Perturbations for material-dependent tallies (GWM/LLC/JSH);
 □ ENDF/B-VI extensions (MCW);
 □ Electron physics enhancements (upgrade to ITS3.0²) (KJA/HGH);
 □ Weight window enhancements (JSH/JAF); and

1.2. Guarantee

MCNPX is guaranteed. We are so confident of the quality of MCNPX that we will pay \$20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. We also will pay a brand new \$2 bill for any error in MCNPX that has been inherited from its constituent codes³.

☐ Distributed memory multiprocessing (GWM).

MCNPX has better quality than MCNP4C3. First, it corrects many MCNP4C3 problems. Second, cash awards have been earned less frequently with MCNPX than with MCNP4C3 and its predecessors. In the past two years less than 20 MCNPX cash awards have been awarded. A listing of winners is available at http://mcnpx.lanl.gov. MCNPX bugs are described with the newsletter for each MCNPX version.

² J. A. Halbleib, R. P. Kensek, T. A. Mehlhorn, G. D. Valdez, S. M. Seltzer, M. J. Berger, "ITS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes," Sandia National Laboratories report SAND91-1634 (March 1992)

³ Cash Award Fine Print: Offer subject to cancellation or modification without notice. A bug is defined as an error in the source code that we choose to correct. We make awards even for the most trivial or insignificant problems, but not for proposed code enhancements or proposed extended capabilities. Awards given only to the first MCNPX user reporting a problem. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We believe MCNPX and its predecessor codes are the most error-free and robust Monte Carlo radiation transport capabilities, and back them with a cash guarantee.

1.3. Availability

MCNPX 2.4.0 is available from the Radiation Safety Information Computational Center in Oak Ridge, TN, USA: http://www-rsicc.ornl.gov. MXNPX 2.4.0 is also available from the OECD NEA Data Bank (Organization for Economic Cooperation and Development – Nuclear Energy Agency) in Paris, France: http://www.nea.fr.

An essential part of the MCNPX software quality assurance plan is the beta test program. Before a code version goes to RSICC or OECD/NEA it is made available to over 1000 MCNPX beta testers worldwide. MCNPX 2.5.c is available to beta testers on the MCNPX website, http://mcnpx.lanl.gov. To apply for a beta test password and to have access to the latest MCNPX versions, contact Laurie Waters, lssw@lanl.gov.

All beta test, RSICC, and OECD/NEA versions of MCNPX are guaranteed with cash awards.

2.0. USER INTERFACE FOR NEW MCNPX FEATURES

The new MCNPX capabilities involve a number of user interface changes from MCNP4C3 and older MCNPX (2.3.0 and earlier) versions. These changes are mostly extensions of existing input cards.

2.1. PHYS Changes

2.1.1. Neutrons

PHYS:N EMAX EAN IUNR DNB TABL FISM RECL

EMAX = upper energy limit (default = 100 MeV)

EAN = analog capture below EAN; implicit capture above EAN (default = 0 MeV)

IUNR = unresolved resonance range probability table treatment

= 0/1 = on/off (default = 0) when unresolved data are available

DNB=delayed neutrons from fission.

- -1 = analog production of delayed neutrons from fission (default)
- 0 = treat prompt and delayed neutrons as prompt
- n =biased production: produce up to n delayed neutrons per fission (n > 0 disallowed in KCODE)
- TABL = use data tables below TABL; physics models above TABL
 - = -1 (default) (Mix and Match) When tables are available use them up to their upper limit and use physics models above.

FISM = fission multiplicity

- = 0 (default) MCNP treatment. The number of neutrons per fission is the integer above or below •. If = 2.7, then the number of neutrons will be 2 30% of the time and 3 70% of the time.
- = FWHM: sample Gaussian with full-width half-maximum of FWHM about •

= -1 : sample Gaussian with FWHM appropriate for fissioning nuclide (recommended)

RECL = light ion recoil. Produce 0 < RECL < 1 light ions (h, d, t, s, a) at each elastic scatter with light nuclei (H, D, T, 3 He, 4 He). The ionization potential is accounted for, and the proper two-body kinematics is used (with neutron free-gas thermal treatment if appropriate) to bank the created particles with the proper energy and angle. MODE n h d t s a ... is required to produce 1 light ions (h, d, t, s, a). CUT:x 2J 0 for x = h, d, t, s, a is recommended so that the low-energy recoil ions produced are not killed by energy cutoff.

2.1.2. Protons

PHYS:H EMAX EAN TABL | ISTRG | RECL

EMAX = upper energy limit (default = 100 MeV)

EAN = analog capture below EAN; implicit capture above EAN (default = 0 MeV)

TABL = use data tables below TABL; physics models above TABL

= -1 (default) (Mix and Match) When tables are available use them up to their upper limit and use physics models above.

J = jump (unused)

ISTRG = charged particle straggling control

- = 0 Vavilov (default, best)
- = 1 Continuous slowing down approximation
- = -1 old MCNPX 2.2.4 method

J = jump (unused)

RECL = light ion recoil. Produce 0 < RECL < 1 light ions (h, d, t, s, a) at each elastic scatter with light nuclei (H, D, T, 3 He, 4 He). The ionization potential is accounted for, and the proper two-body kinematics is used to bank the created particles with the proper energy and angle. MODE h d t s a ... is required to produce light ions (h, d, t, s, a). CUT:x 2J 0 for x = h, d, t, s, a is recommended so that the low-energy recoil ions produced are not killed by energy cutoff. Note that protons colliding with hydrogen to produce more protons can produce an overwhelming number of protons; caution is required and RECL < 1 may be needed.

2.1.3. Charged particles

PHYS:x EMAX 3J ISTRG

EMAX = upper energy limit (default = 100 MeV)

J = jump (unused)

ISTRG = charged particle straggling control

- = 0 Vavilov or Prael's new straggling model, which is an energy correction addressing stopping powers. (default, best)
- = 1 Continuous slowing down ionization model

= -1 old MCNPX 2.2.4 method

2.2. MX Card: Mix-and-Match Nuclide Replacement

The new MCNPX MX card enables materials substitution for different particle types. It is an extension of, and replacement for, the MPN card for photonuclear data:

```
MXn:p zaid1 zaid2 ...
where n = material number of an Mn card that MUST precede the MXn card;
 p = particle type (n, p, h)
zaidn = replacement nuclide for the nth nuclide on the Mn card.
```

Only particle types n (neutron), p (photonuclear), and h (proton) are allowed on the MX card. No substitutions are allowed for photoatomic (p) and electron (e) data because those data sets are complete. The MXn:P card is an exact replacement of the MPNn card and specified photonuclear nuclide substitutions (library type u.) zaidn = 0 is allowed on MXn:P (photonuclear substitution) to specify no photonuclear data for a specific photoatomic reaction. zaidn = model is allowed on the MXn:N and MXn:H (neutron and proton substitution) to allow models to be mixed with tabular data. As an example, consider the following input file:

```
mode n h p
phys:p 3j 1
          1002 1
                      1003.61
m1
                                   6012 1
                                               20040 1
                                                            nlib .24c
                                   6000
mx1:n
                      model
                                               20000
mx1:h
         model
                      1001
          6012
mpn1
                      0
```

MCNPX will issue the following warnings:

```
warning. MPNn will soon be obsolete. use MXn:p instead.
warning. photonuclear za = 6012 different from nuclear za = 1002
warning. photonuclear za = 0 different from nuclear za = 1003
```

Note that models will be used for neutron tritium and proton deuterium. The MPN card still works but has a warning. The mixing and matching is summarized in Print **Table 101:**

1particles and energy limits							pri	print table 101			
part	icle t	ype	particle cutoff energy	maximum particle energy	smallest table maximum	largest table maximum	always use table below	always use model above			
1	n	neutron	0.0000E+00	1.0000E+37	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02			
2	p	photon	1.0000E-03	1.0000E+02	1.0000E+05	1.0000E+05	1.0000E+05	1.0000E+05			
9	h	proton	1.0000E+00	1.0000E+02	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02			

2.3. COINC Card: ³He Coincidence Modeling

Helium-3 coincidence detectors may now be modeled using the new COINC card and fission multiplicity (PHYS:N card, 6^{th} entry). The COINC card is:

COINC i1 i2 ...

Where i1, i2, ... are cell numbers of ³He coincidence counting cells. For each cell listed the captures and moments will be output in Print Table 118:

1neutron captures on helium-3, moments and multiplicity distributions by cell. print table 118
cell 23:

neutron captures on 3he												
			cap	tures	C	aptures		mult:	iplicit	y fractions		
	hist	ories	by numb	er	by we	eight	by r	number		by weight	eı	rror
captures =	0	7784		0 (0.00000	E+00	7.7840	00E-01	7	7.78400E-01	0.0	0053
captures =	1	1586	15		1.58600	E-01	1.5860	00E-01	1	58600E-01	0.0	0230
captures =	2	370	7	40 '	7.40000	E-02	3.7000	00E-02	3	3.70000E-02	0.0	0510
captures =	3	167	5	01 !	5.01000	E-02	1.6700	00E-02	1	67000E-02	0.0	0767
captures =	4	51	2	04 :	2.04000	E-02	5.1000	00E-03	5	5.10000E-03	0.1	1397
captures =	5	20	1	00 :	1.00000	E-02	2.0000	00E-03	2	2.00000E-03	0.2	2234
captures =	6	10		50 (5.00000	E-03	1.0000	00E~03	1	00000E-03	0.3	3161
captures =	7	4		28 2	2.80000	E-03	4.0000	00E-04	4	.00000E-04	0.4	4999
captures =	8	5		40 4	1.00000	E-03	5.0000	00E-04	g	5.00000E-04	0.4	4471
captures =	9	2		18 :	1.80000	E-03	2.0000	00E-04	2	2.00000E-04	0.7	7070
captures =	11	1		11 :	1.10000	E-03	1.0000	00E-04	1	.00000E-04	0.9	9999
total		10000	32	88	3.28800	E-01	1.0000	00E+00	1	.00000E+00	0.0	0235
							_					
factor	rial m	noments		by	number		k	oy wei	ght			
	3he			3.288001	7 O1 O	0225	2 2000	10E 01	0.0235	:		
3ho/	3he-1	1/21		1.878001					0.023			
3he (3he			2.1	1.524001					0.1719			
3he (3he-1)				1.37300					0.3026			
3he (3he-1)		•	• •	1.15800					0.4428			
3he (3he-1)			• •	8.08000					0.5956			
			• •									
3he(3he-1)				4.460001					0.7497			
3he (3he-1)				1.880001					0.8803			
3he (3he-1)			-,,-	5.700001					0.9652			
3he (3he-1)				1.100001					0.9999			
3he(3he-1)		(3he-	10)/11!	1.000001	s-04 0.	9999	1.0000	JUE-U4	0.9999	9		

Coincidence counting works only for neutron problems run in a completely analog mode with fission multiplicity and analog capture (PHYS:N J 100 3J-1) or CUT:N 2J 0 0) and NO variance reduction. The ³He captures and moments can be compared to Print Table 117 which has the spontaneous fission source and induced fission summaries of fission neutrons and moments.

2.4. SDEF Source Specifications

2.4.1. Particle Type Specification

The source particle type now may be specified on the SDEF card by its symbol:

SDEF PAR=h

2.4.2. Positron Sources

Positron sources may now be specified:

```
SDEF PAR = -e or SDEF PAR = -3.
```

Note that positron physics in MCNPX, just as with MCNP and the Integrated Tiger Series (ITS), is identical to electron physics except for positron annihilation. Electrons below the energy cutoff are terminated, whereas positrons below the energy cutoff produce annihilation photons. Also, the positrons have a positive charge and may be tallied using the FT card ELC option.

2.4.3. Repeated Structures Source Specifications

The CEL source specification for repeated structures geometries is now consistent with the tally specification. The old MCNP4C specification still works, but the new one is

```
SDEF CEL=d3 POS=0 6 0 EXT=d1 RAD=d2 AXS= 0 1 0
SI3 L (1<10[0 0 0]<11) (1<10[1 0 0]<11) (1<10[2 0 0]<11)
(1<10[0 1 0]<11) (1<10[1 1 0]<11) (1<10[2 1 0]<11)
```

2.4.4. Spontaneous Fission Sources

Spontaneous fission may be specified as a source.

```
SDEF PAR = sf CEL = ...
```

There are 18 available nuclides: ²³²Th, ²³²U, ²³³U, ²³⁴U, ²³⁵U, ²³⁶U, ²³⁶U, ²³⁷Np, ²³⁸Pu, ²³⁹Pu, ²⁴⁰Pu, ²⁴¹Pu, ²⁴¹Pu, ²⁴²Cm, ²⁴²Cm, ²⁴²Cm, ²⁴³Bk, and ²⁵²Cf.

Cells are sampled according to the usual SI and SP distributions. If more than one spontaneous fission nuclide is in a source cell, the fissioning nuclide will be chosen proportionately to the product of its atom fraction and the spontaneous fission yield for each nuclide. If no spontaneous fission nuclide is found in a specified source cell, the code exits with a bad trouble error, "spontaneous fission impossible."

The number of spontaneous fission neutrons is then sampled. The spontaneous fission multiplicity data of Ensslin is used. The energies are sampled from a Watt spectrum with appropriate spontaneous fission parameters for the selected nuclide. Presently, only the first spontaneous fission neutron from each history is printed. If the spontaneous fission samples a multiplicity of zero --- that is, no neutrons for a given spontaneous fission --- then the history is omitted from the first 10 history list of Print Table 110. The number of source particles is the number of spontaneous fission neutrons, which will be • times the requested number of source histories on the NPS

card. Presently all summary and tally normalization is by source histories, which is the number of spontaneous fissions, not the number of spontaneous fission neutrons.

Fission multiplicity for induced fissions (6h entry, PHYS:N card) is automatically turned on with the default width (FISM = -1 = nuclide dependent) If FISM > 0 on the PHYS:N card, then that value will be used. Multiplicity and moments are printed in Print Table 117 for both spontaneous and spontaneous + induced fissions.

2.5. Tallies

2.5.1. Expanded Cosine Specification

Cosines may now be specified in degrees. They may also now be specified with flux tallies as

```
*C2 150 120 90 60 30 0 .
```

The * on the C2 card interprets cosines as in degrees. Entries must be such that the cosine is monotonically increasing.

2.5.2. DF card: Default Dose Functions

The DE/DF dose function cards are unchanged, but now have extensions. As before, dose conversions may be input as a table. Note that the interpolation int = \log or int = \log now be placed anywhere and that n = tally number, which implies particle type.

```
DEn E1 E2 int E3 ...
DFn F1 int F2 F3 ...
```

The dose conversion capability is extended to provide standard default dose functions. These are invoked by omitting the DE card and using keywords on the DF card:

```
DFn iu=j fac=F int ic=I,
```

where the following entries are all optional.

```
    iu = 1 = US units (rem/h)
    iu = 2 = international units (sieverts/h)
    Default: iu = 2 international units (sieverts/h)
```

fac = normalization factor for dose (acr is also accepted instead of fac).

fac = -1 = normalize results to Q = 20 by dividing the parametric form of Q [5.0+17.0*exp(-(ln(2E))*2/6)] from ICRP60 (1990), paragraph A12.

fac = -2 = apply LANSCE albatross response function.

Default: fac = 1.0.

int = "log" or "lin" results in "log" or "lin" interpolation of energy; the dose function is always linear. That is, "lin" results in "linlin" interpolation, and "log" results in "loglin" interpolation.

Default: for ic = 10, 40: \log

for ic = 20,31-39: recommended analytic parameterization.

ic = i = standard dose function.

i neutron dose function

10 = ICRP-21 1971

20 = NCRP-38 1971, ANSI/ANS-6.1.1-1977

31 = ANSI/ANS-6.1.1-1991 (AP anterior-posterior)

32 = (PA posterior-anterior)

33 = (LAT side exposure)

34 = (ROT normal to length and rotationally symmetric)

40 = ICRP-74 1996 ambient dose equivalent

i photon dose function

10 = ICRP-21 1971

20 = Claiborne & Trubey, ANSI/ANS 6.1.1-1977

31 = ANSI/ANS-6.1.1-1991 [AP (anterior-posterior)]

32 = PA (posterior-anterior)

33 = (LAT side exposure)

34 = (ROT normal to length and rotationally symmetric)

35 = (ISO isotropic)

Default: ic = 10

Examples:

DF4

DF0 ic 40 iu 1 lin fac 123.4

DF1 iu=2 acr=-2 log ic=34

2.5.3. Photonuclear and Proton Reaction Multipliers

Photonuclear and proton cross sections may be used in tally multipliers on the FM card. For example,

M102 92235 1 pnlib=27u F2:P 1 FM2 (-1 102 18 1018)

Photonuclear cross-section reaction numbers are all positive, unlike the photoatomic reaction numbers which are negative. The principal photonuclear cross sections are: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, $>4 = \text{various reactions such as } 18 = (\gamma, f)$. The photonuclear yields (multiplicities) for various secondary particles are specified by adding $1000 \times 1000 \times 100$

Proton reaction numbers are similar to the neutron reaction numbers: all positive. The principal proton cross sections are: $\pm 1 = \text{total}$, $\pm 2 = \text{nonelastic}$, $\pm 3 = \text{elastic}$, $\pm 4 = \text{heating}$, >4 = various reactions. On the LA150H proton library, the only available reaction is mt = 5 and its multiplicities, 1005, 9005, 31005, etc. The multiplicity reaction numbers are specified by adding 1000 x the secondary particle number to the reaction number. For interaction reaction mt = 5, the multiplicities are 1005 for neutrons, 9005 for protons, 31005 for deuterons, etc. The proton multiplicity, mt = 9001, 9004, 9005, etc., is generally available along with the total cross-section and heating number, mt = 1, mt = 4.

It is always wise to plot the desired cross sections first to see if they are available with the expected reaction numbers in the data library. The tally multipliers treat the data the same as the data are treated in transport: the cross section at the lowest energy is extended down to E = 0 for protons with mt < 0; the cross section at the highest energy of the table is extended to $E = \infty$ for proton interaction cross sections with mt < 0 and for photonuclear interaction cross sections, mt < 1000. These extrapolations can be seen in the cross-section plots.

2.6. Geometry Plots

The new plotting capabilities are accessible via either the interactive geometry plot capability or the command/prompt interface.

2.6.1. I,J,K Lattice Index Labeling

The i,j,k lattice indicies of repeated structures/lattice geometries may now be used as plot labels in geometry plots as illustrated in Figure 1.

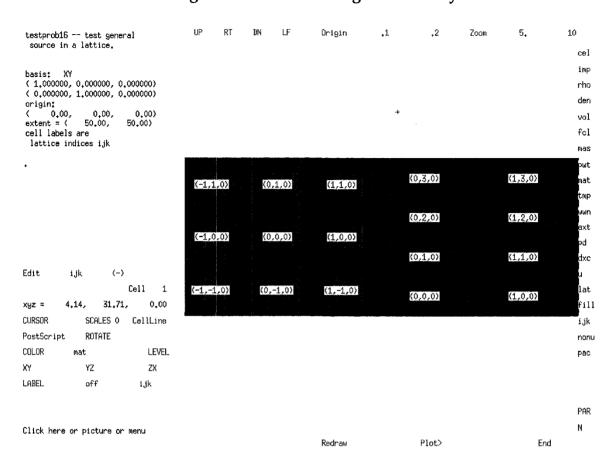


Figure 1: Lattice Indexing in Geometry Plot

If the level (LEVEL command or button) is not a lattice cell level, then the indicies will be for the next lattice in a higher level. To get the lattice index labels, choose ijk as the edit quantity by clicking ijk in the right margin. Then click the send entry after LABEL so that it reads "LABEL off ijk". For command/prompt plotting, enter "Label 0 1 ijk"

2.6.2. 64-Color Plotting and Coloring by Cell Parameters

MCNP4C3 has 7 plotting colors; MCNPX now has 64-color plotting. Coloring of geometry plots may be for any cell parameter. MCNP4C colored geometry plots by material only, giving a different color to each material number. MCNPX can now color geometry plots by any cell quantity. Each cell can have a different color, or each repeated structure level or universe can have a different color. Logarithmic shading of importances, weight windows, and summary information is automatic. If a superimposed weight window mesh is used, coloring may also be by the value of the mesh weight windows.

In the interactive capability, the "SCALES n" button has been moved up two lines (after the cursor) to make room for a larger "COLOR name" button. The default is "COLOR mat", which colors problem cells by the program material number. This button must be

clicked to get "COLOR off" (black and white) and then clicked again to color by whatever parameter is listed after the "Edit" button. For example, in the right margin, click "cel", which will make the "Edit" quantity "cel". Next, click "COLOR" so that it says "COLOR cel"; on the next plot, the color shades will be by program cell number.

For command/prompt plotting, enter

PLOT> label 0 1 rho;

the color command then must be set such as

PLOT> color on

and the coloring will now be by rho, the atom density.

2.7. Tally and Cross Section Plots

2.7.1. Pause Command

The MCNPX geometry plot *PAUSE* command is now extended to tally and cross-section plots. When the word *PAUSE N* is put in a tally plotting COM input file, the picture will display for *N* seconds. If the command *PAUSE* (without the *N*) is in the COM file, then the display will hold until a key is struck.

2.7.2. Photonuclear Cross-Section Plots

MCNPX can plot photonuclear data in addition to the photoatomic data of MCNP.

Photoatomic reaction numbers are all negative: -1 = incoherent, -2 = coherent, -3 = photoelectric, -4 = pair production, -5 = total, -6 = heating. For the MCNPX photonuclear cross-section plotting, the reaction numbers are all positive. The principal photonuclear cross sections are: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, >4 = various reactions such as 18 = (γ,f) . The photonuclear yields (multiplicities) for various secondary particles are specified by adding 1000 x the secondary particle number to the reaction number. For example, 31001 is the total yield of deuterons (particle type d = 31); 34001 is the total yield of alphas (particle type α = 34); 1018 is the total number of neutrons (particle type n = 1) from fission. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as m = 99 and MCNPX will list the available photonuclear reactions and the available yields such as 1018, 31018, 34018. Entering a bad nuclide, m = 12345.67m, will cause MCNPX to list the available nuclides.

Figure 2 illustrates a photonuclear cross-section plot of the total photonuclear cross section, mt = 1, for material 11 and its constituents, carbon and lead.

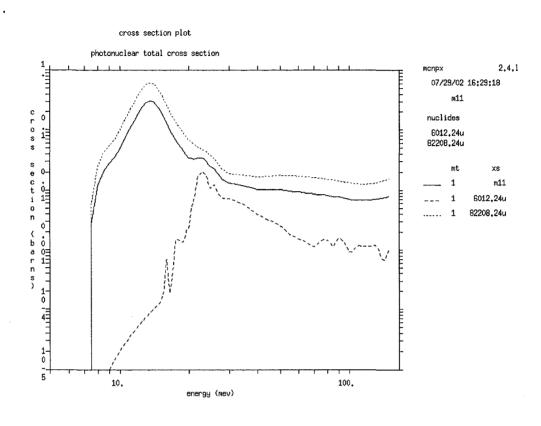


Figure 2: Photonuclear Cross Section Plot

2.7.3. Proton Cross-Section Plots

MCNPX can now plot proton cross-sections. The reaction numbers are similar to the neutron reaction numbers: all positive. The principal proton cross sections are: $\pm 1 = \text{total}$, $\pm 2 = \text{nonelastic}$, $\pm 3 = \text{elastic}$, $\pm 4 = \text{heating}$, > 4 = various reactions. On the LA150H proton library, the only available reaction is mt = 5 and its multiplicities, 1005, 9005, 31005, etc. The multiplicity reaction numbers for interaction reaction mt = 5 are 1005 for neutrons, 9005 for protons, 31005 for deuterons, etc. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99, and MCNPX will list the available proton reactions and the available yields such as 1005, 32001, 34002, etc. The proton multiplicity, mt = 9001, 9004, 9005, etc., is generally available along with the total cross-section and heating number, mt = 1, mt = 4. Entering a bad nuclide, mt = 12345.67h, will cause MCNPX to list the available proton nuclides.

2.7.4. Annoying Bell

The bell that "beeped" when plots were finished has been disabled. In ancient times one had to wait forever to get plots up on the screen and so the bell announced that the plot was ready. Now plotting is so fast that the bell is annoying and unneeded.

2.8. Other Capabilities

2.8.1. Logarithmic Interpolation

Logarithmic interpolation is now allowed on all input cards where lists of numbers are given. It is similar to the IJMR interpolation. For example,

E0 1.e-3 6log 1.e4

is interpreted as

E0 .001 .01 .1 1 10 100 1000 10000 .

2.8.2. Changes in Installation/Compilation

The autoconfiguration has been significantly upgraded for MCNPX installation and compilation. Fortran90 is now the default, so on unix systems it is no longer necessary to configure with:

configure -with-FC=f90 -with-CC=cc

Instead, simply enter:

configure

2.8.3. MPI Mutiprocessing

To compile MCNPX with MPI it is necessary to use the new "MPI" compilation/configuration directive:

Configure -with-FFLAGS="-DMULTP=1-DMPI=1"

To run an MCNPX problem with MPI, all one must do is start the MPI daemon (which is typically already running on most systems) and then start MCNPX using "MPIRUN". An example is:

mpirun -np 4 mcnpx inp=gwm na=gwm1. ...

This is quite different than PVM, which required knowledge about setting certain links, environment variables, and the PVM console commands. The PVM execution command is like:

Mcnpx inp=gwm n=gwm1. tasks=-12x16

3.0. DESCRIPTION OF NEW MCNPX 2.5.C FEATURES

The princ	ripal MCNPX 2.5.c new features are:
	MPI multiprocessing (JL/GWM);
	I,J,K lattice indexing in geometry plots (JSH),
	Enable weight window generator in physics model region (FXG/JSH);
	Enable exponential transform in physics model region (FXG/JSH);
	Extend neutron model physics below 20-MeV (JSH);
	3-He coincidence detector modeling (HGH/JSH);
	F90 Autoconfiguration (TLR);
	Corrections/enhancements/extensions.

3.1. MPI Multiprocessing

MCNPX now supports distributed memory multiprocessing for the entire energy range of all particles with both PVM and MPI. MPI is the Message Passing Interface standard from Argonne National Laboratory, http://www-unix.mcs.anl.gov/mpi/. PVM is Parallel Virtual Machine, http://www.csm.ornl.gov/pvm/pvm home.html/, from Oak Ridge National Laboratory. Fault tolerance and load balancing are available, and multiprocessing can be done across a network of heterogeneous platforms. Threading may be used for problems run in the tabular data region only.

Testing to date on a Linux cluster shows that the MPI version of MCNPX is slightly slower than that of the PVM; however, MPI can make use of the native high-speed interconnects (e.g., Myrinet) rather than just Ethernet. PVM cannot make use of these speedy interconnects as it is forced to use TCP/IP.

The MCNPX 2.5.c MPI capability dynamic buffering for the MPI implementation. This is a significant advantage over PVM other implementations which use a fixed buffer size (the PVM buffer size is controlled with an environment variable - which most people know nothing about). The initial buffer size is set to 10 Mbytes and the maximum number of increases is 10, resulting in an upper limit of 100 Mbytes. These values are set via parameters which are easily modified in module ESSAGE_PASSING. Testing included varying these significantly to ensure answers would not change

MPI enables parallel computations on PC Windows. PVM does not yet support Windows 2K.

MPI only requires "freeware" software, as did PVM. The MPICH product can be downloaded from ANL and installed on either Windows or Unix platforms. On Unix platforms, one must take care to produce Fortran 90 versions of the libraries and not the default Fortran 77 ones. On Windows, one does not even need to build the MPI libraries as one can simply download and install the pre-built ones. So far MCNPX MPI has been tested on Linux, SGI, and Windows PC.

With MPI, MCNPX execution is much easier. All one must do is start the MPI daemon (which is typically already running on most systems) and then start MCNPX using "MPIRUN". An example is:

mpirun -np 4 mcnpx inp=gwm na=gwm1. ...

This is quite different than PVM, which required knowledge about setting certain links, environment variables, and the PVM console commands.

MPI Drawbacks:

As with most new features, there are still some problems with the MPI implementation. Most likely these will be addressed in the near future as we gain more experience with MPI:

- (1) On Unix platforms, MPI adds 4 arguments to the command line. Most MPI codes either don't take input from the command line or find a way to accept these new arguments. For now, MCNPX simply subtracts 4 from the number of command-line arguments and thus ignores these system-dependent arguments (they are always added to the end of the argument list). A couple of other options are: (a) ignore unrecognized command-line arguments (right now we give a fatal error); or (b) add the logic to process these new arguments.
- (2) Interrupts don't work when running with multiple processes (they do for sequential execution). It appears that MPIRUN captures this interrupt and kills the job (on all platforms). There may be an MPIRUN option to avoid this, but we haven't found it yet.

3.2. I,J,K Lattice Indexing in Geometry Plots

It is now possible to label repeated structures/lattices with their i,j,k indicies in geometry plots. See Section2.6.1.

3.3. Weight Window Generator Improvements

The weight window generator variance reduction capability has been extended to the MCNPX physics model region for both neutral and charged particles. Both cell-based and mesh-based weight windows can now be generated for high-energy problems.

MCNPX now allows cell-based weight windows and importances to be used in conjunction with mesh based weight windows. Previously, all WWINP file weight windows had to be used if available and importances were used otherwise. Now, WWINP weight windows are used only if 5th WWP entry is negative; otherwise cell-based windows or importances from input file are used. In particular, if a mesh-based

window is bad in the WWINP file, it may now be ignored and importances or cell-based windows from the input file may be used instead.

Whenever there are multigroup weight window generated, MCNP and MCNPX generate a one group weight window file as well, WWONE. Now the WWONE file includes one group windows for all particles regardless of how many weight window generator groups, if any, those particles had. Previously the WWONE file was worthless if some particles had one group windows generated and other particles generated multigroup windows.

3.4. Exponential Transform in Physics Model Region

The exponential transformation variance reduction technique is now available for neutral particles in the physics model region of MCNPX. Note that the exponential transform should not be used without weight windows.

3.5. Extend Neutron Model Physics Below 20 MeV

MCNPX may now use neutron models below 20 MeV. This is useful for nuclides where there is no table data, such as germanium in a BGO detector. It is also useful for running pulse height tallies and other analog problems where data table (n,2n) reactions are not correlated whereas the model physics reactions are all correlated. Finally, it is useful for comparing the models to the data tables. A major report is now available comparing physics model and data table results as part of the Mix and Match documentation.⁴

3.6. ³He Coincidence Detector Modeling

MCNPX now has a ³He neutron coincidence detector model. See Section 2.3. It works in conjunction with fission multiplicity and analog capture (Section 2.2.1) and optionally with spontaneous fission sources (Section 2.4.4).

Multiplicity counting⁵ is a nondestructive assay technique for fissionable materials. Neutron coincidence counting looks for groups of neutrons that are close together in time, within the coincidence resolving time or "gate width" of the electronics package. In practice, multiplicity data analysis is not based directly on the observed multiplicity distribution but on the moments of the distribution. The factorial moments, ν_k , of a neutron multiplicity distribution emitted by a multiplying sample are ⁶⁷

⁴ John S. Hendricks, "MCNPX Model/Table Comparison," Los Alamos National Laboratory Report, LA-14030 (March 2003)

⁵ N. ENSSLIN, W. C. HARKER, M. S. KRICK, D. G. LANGNER, M. M. PICKRELL, J. E. STEWART, "Application Guide to Neutron Multiplicity Counting," *Los Alamos National Laboratory report* LA-13422-M (November 1998)

⁶ K. BOEHNEL, "The Effect of Multiplication on the Quantitative Determination of Spontaneously Fissioning Isotopes by Neutron Correlation Analysis," *Nuclear Science and Engineering*, **91**, 114 (1985)

$$v_1 = \bullet v P(v), v = 1, \max$$

$$v_2 = \bullet v (v - 1) P(v), v = 2, \max$$

$$v_3 = \bullet v (v - 1) (v - 2) P(v), v = 3, \max$$

$$v_k = \bullet v! P(v) / (v - k)!, v = k, \max$$

The MCNPX fission multiplicity and ³He coincidence counting capabilities of MCNPX enable direct comparisons with measurements.

Fission multiplicity in MCNPX samples the correct number of fission neutrons to emerge from a fission event. Previous MCNPX/MCNP versions simply emitted the nearest number of fission neutrons to ν_{avg} . Thus, for ν_{avg} = 2.7, two neutrons would be emitted 30% of the time and three neutrons would be emitted 70% of the time. Now the correct number, from 0 to 11, of fission neutrons is emitted at each fission and both the multiplicity distribution and moments are tabulated for all fissions. The number of fission neutrons from each fission event is sampled from the appropriate Gaussian distribution about ν_{avg} .

The coincidence counting model simply counts the analog capture of neutrons by ³He in geometric cells specified on the COINC card. These captures are then tabulated along with the capture moments. Comparison of the capture moments and fission multiplicity moments enables comparison with measurements.

The following table compares MCNPX calculations to measurements for Californium sources in an Epithermal Neutron Multiplicity Counter (ENMC). The table shows a straight comparison between counting rates for singles, doubles, and triples (moments). The experimental values have been corrected for dead time and gate width.

⁷ W. HAGE, D. M. CIFARRELI, "Correlation Analysis with Neutron Count Distributions in Randomly or Signal Triggered Time Intervals for Assay of Special Nuclear Materials," *Nuclear Instruments and Methods*, **A236**, 165 (1985)

Compariso	on of Measu	rement/MCNPX						
MCNPX Calculated Count Rates								
	S	D	T					
Cf-10	159835	99959	37075					
Cf-11	296568	185470	68792					
Cf-12	567456	354881	131627					
		ENMC Measured	d Rates					
Cf-10	160788	100573	36426					
Cf-11	297647	186006	68173					
Cf-12	569117	355386	130467					
		Measurement/Cal	lculation					
Cf-10	1.0060	1.0061	0.9825					
Cf-11	1.0036	1.0029	0.9910					
Cf-12	1.0029	1.0014	0.9912					
Average	1.004	1.003	0.988					
St. Dev.	0.002	0.002	0.005					

3.7. Fortran90 Autoconfiguration

The MCNPX autoconfiguration code installation and compiling capability has been significantly revised. The F90 compiler is now the default on all platforms and it is no longer necessary to declare F90 at the configure step. See Sections 2.8.2 and 2.8.3. The directories and compile directives have been revised to prepare for the imminent integration of the INCL (Cugnon/Schmidt) physics model.

Fortran90 provides improvements in code modularity, standardization of functions such as timing across platforms, and compiler reliability. F90 will run more slowly on some systems. Specifically, we have eliminated equivalences as a means of dynamic storage allocation by using F90 pointers and allocable arrays. We have replaced most common calls with F90 modules. The code will compile in both free and fixed F90 formats.

MCNPX can be modified by patches, and as much of the MCNP4C coding as possible has been preserved so that MCNP4C patches can be applied directly to MCNPX.

Continuing improvements in the F90 structure are ongoing, especially where they concern physics modules that have been brought into the code.

3.8. Corrections/Enhancements/Extensions

3.8.1. Some Significant Problems

The following problems could cause wrong answers.

3.8.1.1. Dynamic Memory Allocation Error

The following problems have occurred with some compilers on some systems, notably the Sun Solaris Forte 6.2 compiler:

- ✓ Compilation errors preventing compilation;
- ✓ Inability to continue runs;
- ✓ Overwriting of memory.

Consequently, we have reallocated dynamic memory to prevent arrays from ever having zero length. Evidently zero-length arrays has always been possible on older compilers and systems.

3.8.1.2. Physics Model Heating Wrong

In all previous versions of MCNPX (and probably LAHET as well) the heating in the physics model energy range only is multiplied by the particle weight squared. Thus if the weight is not exactly one, then the heating is wrong. Fortunately, most problems use a source weight of one and there is seldom variance reduction in the physics model region. To see if your problems were affected, try a source weight of SDEF WGT=1000. If your heating tallies increase by a factor of 1000, then everything is OK. If they increase by a factor of 1000000 then this bug affected you.

3.8.1.3. Light-Ion Recoil Errors

In previous versions light ion recoil was off by a factor of the atomic weight ratio. Thus recoil of protons was correct, but recoil of other light ions was wrong. \$20 awarded to Martyn Swinhoe (LANL, NIS-5) (D-10:JSH-2003-034). Also, light-ion recoil bias, when RECL on the PHYS:N card 7th entry was not 0 or 1, resulted in wrong particle weights. \$20 Martyn Swinhoe (NIS-5) (D-10:JSH-2003-030)

3.8.1.4. MDATA Binary Files for Mesh Tallies

The binary format MDATA file used to make mesh tally plots was improperly normalized in KCODE and SSR problems. \$20 awarded to Bernard Verboomen (SCICEN, Belgium) (D-10:JSH-2003-036)

3.8.2. Irritating Problems

The following problems do not cause wrong answers. In some cases MCNPX will crash and in others the desired functionality is simply absent.

3.8.2.1. SPABI Failure

The SPABI capability (secondary particle production biasing) simply did not work for some compilers because an integer function had a floating point name. Answers were correct, just not biased as desired. Also, all previous MCNPX versions put SPABI roulette in the "photon production from neutrons" summary table bin which usually caused unbalanced summary tables. Now the roulette shows up in "energy importance" for all particles.

3.8.2.2. 32-bit SGI Compiler Error

An error in some compilers for 32-bit SGI machines caused an out-of-range error. We have built in a workaround in MCNPX even though this is an SGI error that causes a crash, not an MCNPX error.

3.8.2.3. Occasional Crashes for Some Data Libraries

MCNPX sometimes crashed if angular distributions from the nuclear data tables were in tablular format. Affected only certain data libraries in certain energy regimes.

3.8.2.4. CEM Fails for Light Nuclei

CEM goes into an infinite loop for light nuclides, A < 5. MCNPX25c is changed to use Bertini for A < 5, and CEM for 5 < A < 10 (though Stepan Mashnik says CEM should not be used for A < 10. Photonuclear production is now turned off for A < 5.

3.8.2.5. Gridconv Typo

When running the auxiliary program GRIDCONV to generate mesh tallies, the incorrect question, "Do you what" was changed to "Do you want" in the user interface.

3.8.3. Enhancements

The following enhancements were made to MCNPX 2.5.c in addition to the major new capabilities listed above.

3.8.3.1. Spontaneous Fission, Fission Multiplicity, and ³He coincidence

✓ The source weight in the summary table and 1st 50 histories printed in Print Table 110 are fission neutrons, not fissions.

- ✓ The summary of spontaneous fission and induced fission multiplicity, Print Table 117, computes and lists the estimated error.
- ✓ The summary of ³He capture, Print Table 118, computes and lists the estimated error.
- ✓ Spontaneous fission has been extended from 6 to 18 fission nuclei.

3.8.3.2. Enabling More Histories

An integer overflow has been fixed so that more histories can be run. With the new MPI and PVM parallel capabilities more and more particles are being run.

3.8.3.3. **CEM and LEB**

The LEB parameter can now be increased when running with CEM. Pointed out by Paul Goldhagen, USDOE (New York).

4.0. FUTURE WORK.

- Intra Nuclear Cascade Lei ge (INCL) (Cugnon/Schmidt) physics model.
- Plotting of physics model total and absorption cross sections.
- Special features for space applications.
- Forced collisions for neutral particles extended to physics models.
- Secondary particle angle biasing for isotropic distributions.
- Improved high energy physics with the LAQGSM model.
- Multiple source particle types.
- Pulse height tallies with variance reduction.
- Neutral particle perturbation techniques extended to physics model region.
- Interactive tally and cross-section plotting.
- Detectors and DXTRAN for all neutral particles at all energy ranges.
- A capability to continue runs that write HTAPE files
- Integration of HTAPE tallies directly into MCNPX.
- Heavy ion tracking and interactions.

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